NUMERICAL STUDY OF SINGLE COAL PARTICLE COMBUSTION IN O_2/N_2 AND O_2/CO_2 ATMOSPHERES

Wang L.W.*, Karimi N. and Paul M.C.
Systems, Power & Energy Research Division, School of Engineering,
University of Glasgow,
Glasgow G12 8QQ,
UK
*Email: l.wang.4@research.gla.ac.uk

ABSTRACT

This paper reports a modelling work on the existing experimental data of single coal particles combustion process [1,2]. Two kinds of coal particles (a high-volatile bituminous coal / a lignite coal) are injected in a drop-tube furnace, ignited and burned in quiescent O_2/N_2 and O_2/CO_2 atmospheres with oxygen mole fraction varying from 20% to 100%. Ignition delay time, particle life time and particle surface temperature are calculated to analyse the combustion behaviour of the single coal particle. Transient simulations are carried out based on Discrete Phase Model (DPM). The predicted results are in good agreement with the experimental data and give the details of combustion process. Further, predictions of NOx emissions are made to understand the influence of different gas atmosphere and oxygen mole fraction. This includes both thermal-NO_x and fuel-NO_x formation mechanisms. It is argued that the NO_x emissions in both O_2/N_2 and O_2/CO_2 atmospheres are the result of competitions between the maximum particle temperature and the burning time.

INTRODUCTION

Coal is widely used for energy production across the world and pulverised combustion is perhaps the most common technology for utilising coal energy. Despite serious emissions caused by coal combustion, it is still and, most probably, will continue to be amongst the main resources for power generation [3,4]. Coal combustion which involves devolatilization, char combustion and gas phase reactions is a multi-phase, multi-scale and multi-component process [2]. Types of coal and the operation condition of reactors are also the key factors in its combustion behaviour. Further, the complex chemical processes involved in coal combustion need to be explored.

Due to the increasing concerns about global warming, carbon dioxide emission by coal combustion is now a serious issue. Different methods have been developed for carbon capture and storage (CCS) to reduce the CO_2 emission from coal-fired power plants. Pre-combustion capture, post-combustion capture, oxy-fuel combustion and chemical looping are four main CCS technologies [5]. Among these, the oxy-fuel combustion is a near-zero emission technology and the most promising one for power station utilisation [5]. The replacement of air with O_2/CO_2 leads to modified distributions of temperature and species, as well as radiation flux, resulting from the property differences between N_2 and CO_2. This also results in changes in NO_x formation and reduction in the flame temperature [6].

Nitrogen oxides, including nitric oxide (NO), nitrogen dioxide (NO_2), nitrous oxide (N_2O) are mostly produced through the oxidation of the molecular nitrogen in air (thermal NO_x) and the organically bound nitrogen in the coal (fuel NO_x) [7]. NO_x formed from molecular nitrogen and hydrocarbon fragments resulting from the devolatilization process near the reaction zone of flame (prompt NO_x) accounts for less than 5% of the total NO_x formed [8], and is usually neglected in modelling. In a combustion system, including pulverized combustion, the formation and destruction of NO_x emissions are influenced by several factors such as fuel properties and, combustion conditions e.g. temperature of reaction and the fuel–air ratio [9]. Replacing the background gas N_2 by CO_2 can limit the NO_x emissions formed at high temperatures from nitrogen of the combustion air, and then the formation of NO_x is mainly due to the conversion of fuel-N, partially or totally into nitrogen oxides [10].

NOMENCLATURE

K	[kmol/m^{3}s]	Reaction rate
k	-	Reaction rate constant
c	[kmol/m^3]	Concentration
A	-	Pre-exponential factor
E	[J/kmol]	Activation energy
T	[K]	Temperature
R		Universal gas constant
X	-	Mole fraction
a	-	Oxygen reaction order
b	-	Temperature exponent
d	-	Reaction order
e	-	Reaction order

Special characters

α	-	Distribution coefficient

Subscripts

s	Solid
x	Composition of chemical element H
y	Composition of chemical element O
R	Reactant
ox	Oxidant

The effects of O_2/N_2 and O_2/CO_2 gas atmosphere on coal combustion and NO_x emissions have been investigated by a number of authors. Experiments conducted by Rathnam et al. [11] showed that the devolatilization rate was similar in either N_2 or CO_2 at temperatures lower than 1000 K, while it was higher in CO_2 than in N_2 when temperatures exceeded 1000K. These results were confirmed by Al-Makhadmeh et al. [12]. On the other side, different studies show a minor or even a negative effect of CO_2 atmosphere on coal reactivity [13,14]. Experimental studies on NO_x emission characteristics in coal-fired O_2/CO_2 combustion have been performed in the laboratory [15-18]. Okazaki and Ando [15] concluded that the influence of CO_2 on NO emission is negligible despite its high concentration. Furthermore, an effect of the interaction of fuel-N and recycled NO was detected. Moreover, reduction of NO to molecular N_2 due to chemical reaction in the combustion zone is taken as the main reason for the overall decrease (50-80%) in NO during recycling. Hu et al. [16] evaluated three types of coals for a wide range of stoichiometries with the recycling ratio ranging from 0 to 0.4 and concluded that the reduction ratio (RR) increased with the fuel equivalence ratio and recycling ratio. Recently, Dhungel et al. [17] examined NO emission behaviour during oxy coal combustion in a 20 kW electrically heated furnace and concluded that the pathways of NO reduction in oxy-fuel were fundamentally similar to those in air combustion. Mackrory et al. [18] investigated oxy-fuel combustion in a multi-fuel flow reactor (MFR) and found that oxy-fuel combustion can result in lower NO_x emissions than air combustion independent of the reduction of recycled NO_x, which was different from previous studies.

Computational fluid dynamics (CFD), which can effectively integrate turbulent mixing, combustion chemistry, heat transfer and their interactions together has become a very powerful method to understand and simulate the combustion of coal. Kuffa et al. [19] successfully modelled coal gasification in a fluidized bed reactor. Oevermann et al. [20] established a model for simulating wood gasification in a fluidised bed reactor by using the Euler–Euler approach. Useful CFD analyses of oxy-fuel combustion have been successfully performed and reported in literature as well. CFD simulations of lab-scale oxy-coal combustion were carried out by Chui et al. [21] to assist with future pilot scale oxy-fuel combustion experiments and burner scale-up. Wang et al. [22] conducted a comprehensive CFD simulation of a propane-fueled, oxygen-enriched, turbulent, non-premixed jet flame. Zhou and Moyeda [23] performed CFD simulations for process evaluation of oxy-fuel combustion with flue gas recycle in a conventional utility boiler. However, fewer research focused on the whole combustion process of single coal particles, e.g. ignition characteristics, particle temperature, NOx emissions. Moreover, attention on coal combustion under varied gas atmosphere need to be paid.

This paper aims at developing a combustion model considering the different gas–solid behaviours, heat transfer and thermal conversion processes for single coal combustion by using Discrete Phase Model. The work is also concerned with formation of NO_x emissions when burning different kinds of coal under varying oxygen concentration with both N_2 and CO_2 as the background gas.

FUEL PROPERTIES

The proximate and ultimate analysis of the two kinds of coal is shown in Table 1 [1]. The diameter of particles is defined as 80 μm when carrying out numerical simulations as the size of 75-90 μm was used in the experiments [1].

Table 1 Coal Analysis Data

Fuel	PSOC-1451 Bituminous	DECS-11 Lignite
Proximate analysis (received)		
Moisture (%)	2.5	13.2
Volatile (%)	33.6	48.6
Fixed Carbon (%)	50.6	29.8
Ash (%)	13.3	8.4
Ultimate analysis (dry basis)		
C	71.9	66.2
H	4.7	4.0
O	6.9	18.6
N	1.4	0.9
S	1.4	0.7
Ash	13.7	9.6
Heating value dry fuel (MJ/kg)	31.5	25.7

COMBUSTION MECHANISMS

Coal Combustion

Four chemical processes were considered during coal particles combustion: devolatilization, volatile (represented by CH_xO_y) combustion, char (represented by $C_{(s)}$) oxidation and other gas phase reactions.

The particles are heated up and consequently they release moisture (drying process) at first, and then releasing volatiles rapidly (devolatilization process).

In this study, volatiles release is described by the single rate model. It assumes that the rate of devolatilization is first-order dependent on the amount of volatiles remaining in the particle and employs global kinetics. The reaction and its rate constant are:

R1: coal $\rightarrow$ α volatile + (1-α) char

$k_d = A \exp(-E/RT)$

Char formed during devolatilization process is consumed by heterogeneous processes of combustion and gasification and its combustion yields carbon monoxide (CO) and carbon dioxide (CO_2). Heterogeneous reactions can also include the char-H_2O reaction.

R2: $C_{(s)} + O_2 \rightarrow CO_2$

R3: $C_{(s)} + 0.5\ O_2 \rightarrow CO$

R4: $C_{(s)} + CO_2 \rightarrow 2\ CO$

R5: $C_{(s)} + H_2O \rightarrow H_2 + CO$

The combustion rate of char is assumed to be limited by the chemical kinetics because the only reactive species that is included in the gas phase is O_2. Then, the reaction rate K (kmol/m^{3}s) is defined as

$K = k_a\, c_{c(s)}\, c_{o2}$

and k_a is the reaction rate constant given by the Arrhenius type relation:

$k_a = AT^b \exp(-E/RT)$

In the gas phase reactions, as the detailed chemical species in the volatile are not completely understood due to the complexity of the chemical structure of coal, for simplicity in this study, it was generally treated as a single species which varies depending on the type of coal and comprising carbon, hydrogen and oxygen (CH_xO_y) in a ratio determined from the ultimate analysis of coal. For the two kinds of coal (PSOC-1451, DECS-11) used in this study, the volatile gas species are represented as $CH_{2.99}O_{0.24}$ and $CH_{1.48}O_{0.43}$ separately. The homogeneous reaction related to the volatile is as followed:

R6: $CH_xO_y + m\ O_2 \rightarrow CO_2 + n\ H_2O$

Thus, equating the numbers of atoms of each element in the reactants to the number in the products gives:

$m = 1 + x/4 - y/2$

$n = x/2$

And the carbon monoxide (CO) is oxidised to CO_2 according to the following homogeneous reaction:

R7: $CO + 0.5\ O_2 \rightarrow CO_2$

The reaction rates are given as

$K = AT^b \exp(-E/RT)\ [c_R]^d [c_{ox}]^e$

Six chemical reactions are considered totally and a summary of the kinetics data used in the present combustion modelling and the values of d and e are provided in Table 2.

Table 2 Kinetic constants

Reaction NO.	Kinetic parameters			d	e	Ref.
	A	E	b			
R1	3.12E+05	7.4E+07	-	-	-	[24]
R2	4.4	1.62E+08	1	-	-	[24]
R3	1.33	1.47E+08	1	-	-	[25]
R4	0.002	7.9E+07	0	-	-	[26]
R5	0.052	1.33E+08	0	-	-	[26]
R6	1.30E+11	1.26E+08	-	0.5	0.5	[27]
R7	2.119E+11	2.027E+08	-	0.2	1.3	[24]

NOx Formation

The nitrogen forms NO_x emissions via intermediates HCN and NH_3. The reactions related to NO formation and the reduction of NO are as follows:

R8: $HCN + O_2 \rightarrow NO + \ldots$

R9: $NH_3 + O_2 \rightarrow NO + \ldots$

R10: $HCN + NO \rightarrow N_2 + \ldots$

R11: $NH_3 + NO \rightarrow N_2 + \ldots$

The reaction rates are given by De Soete [28] as

$K_8 = A_8 X_{HCN} X_{O2}^{\ a} \exp(-E_8/RT)$

$K_9 = A_9 X_{NH3} X_{O2}^{\ a} \exp(-E_9/RT)$

$K_{10} = A_{10} X_{HCN} X_{NO} \exp(-E_{10}/RT)$

$K_{11} = A_{11} X_{NH3} X_{NO} \exp(-E_{11}/RT)$

The kinetic constants and the oxygen reaction order are shown in Table 3.

NUMERICAL METHOD

The basic geometry used in this study is taken from Khatami et al [1,2]. An axisymmetric computational domain is shown in Figure 1. The coal particles are injected through the origin.

The numerical simulations are performed using an Euler-Lagrange model. The weighted-sum-of-gray-gases model (WSGGM), single-rate devolatilization model and multiple-surface-reactions combustion model (e.g., char-O_2, char-CO_2, and char-H_2O) are used for the modelling. The flow field was solved using the SIMPLE algorithm for velocity-pressure coupling. Gravity is enabled as well when running these numerical simulations. NO_x formation is performed with thermal NO and fuel NO sub-models. The simulations are run on ANSYS FLUENT.

Table 3 Reaction parameters

Reaction NO.	Kinetic constants	
	A	E
R8	1.0E10	2.8E+08
R9	4.0E06	1.33E+08
R10	3.0E12	2.51E+08
R11	1.8E08	1.13E+08
Oxygen reaction order		
Oxygen mole fraction		*a*
$X_{O2} \leq 4.1E-03$		1
$4.1E-03 \leq X_{O2} \leq 1.11E-02^2$		$-3.95-0.9\ln X_{O2}$
$1.11E-02 \leq X_{O2} \leq 0.03$		$-0.35-0.1\ln X_{O2}$
$X_{O2} \geq 0.03$		0

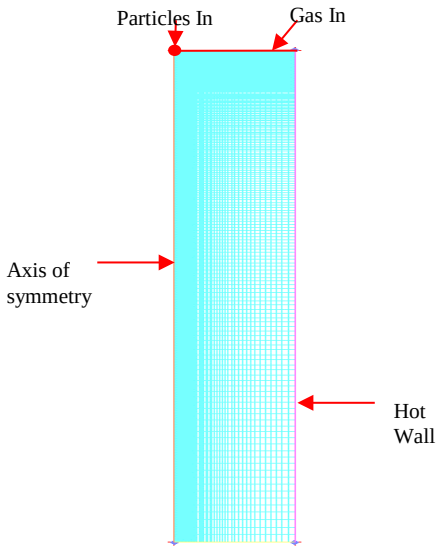


Figure 1 2D axisymmetric geometry with mesh

The coal particle combustion experiments are conducted under a quiescent gas condition (inactive flow, i.e., no injector flow and no furnace flow) and quiescent gas condition is set by turning off the gas flows a few seconds prior to the particle injection [2]. While running numerical simulations, gas injection stops when enabling DPM to inject coal particle. The operating conditions refer to the conducted experiments in ref. [1,2], and are shown in Table 4. Some assumptions are made when running simulations: 1) the coal particles are regarded as spherical in shape and 2) the gas phase are treated as an ideal-gas mixture.

Table 4 Operating Conditions

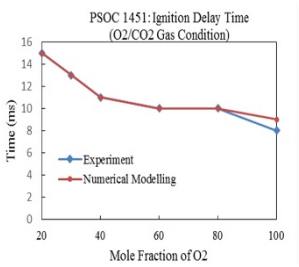
Parameters	Values
Wall Temperature	1400 K
Temperature of injecting gas	1200 K
Velocity of gas	4.55 cm/s
Diameter of particles	80 μm
Initial temperature of particles	1200 K
Velocity of particles	15 cm/s

RESULTS

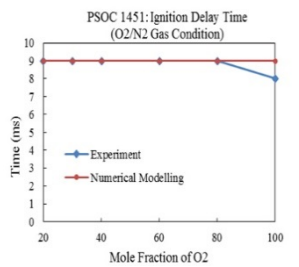
Validation of the Numerical Simulation

Particle ignition delay time, particle life time (sum of particle ignition delay and burnout time) and particle temperature of the two kinds of coal (PSOC-1451 and DECS-11) under quiescent O_2/N_2 and O_2/CO_2 atmospheres with oxygen mole fraction varying from 20% to 100% were measured in the experiments of Khatami et al. [1,2]. Numerical simulations of coal particles combustion were run and data was obtained to compare with experimental one.

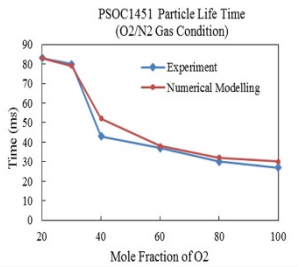
Figures 2(a) and 2(b) show a comparison between the simulated particle ignition delay time and the corresponding experimental data for coal PSOC-1451. The figures show that, apart from the pure oxygen case, the numerical results in other cases spot on the experimental data. Figures 2(c), 2(d) and Figures 2(e), 2(f) give the information of particle life time and particle temperature versus varied oxygen concentration under both N_2 and CO_2 background gas coal PSOC-1451. Once again,



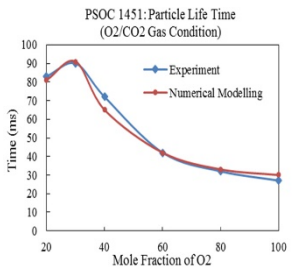
(a) Ignition Delay Time O_2/N_2



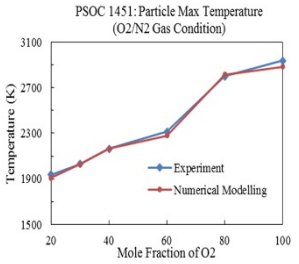
(b) Ignition Delay Time O_2/CO_2



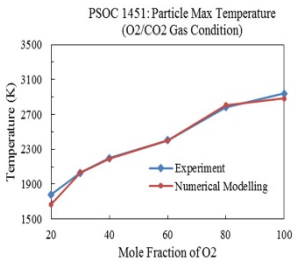
(c) Particle Life Time O_2/N_2



(d) Particle Life Time O_2/CO_2

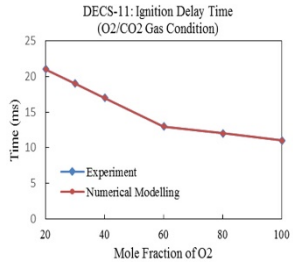


(e) Particle Temperature O_2/N_2

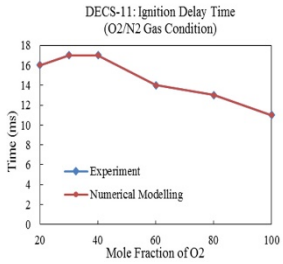


(f) Particle Temperature O_2/CO_2

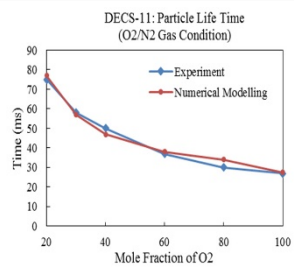
Figure 2 Compared particle ignition time, particle life time and particle temperature versus varied oxygen concentration under both N_2 and CO_2 background gas for coal PSOC-1451.



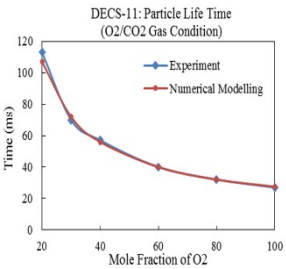
(a) Ignition Delay Time O_2/N_2



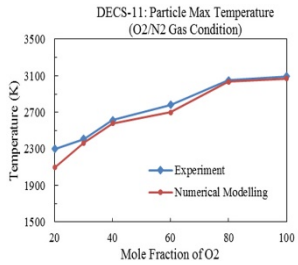
(b) Ignition Delay Time O_2/CO_2



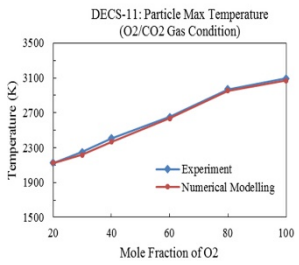
(c) Particle Life Time O_2/N_2



(d) Particle Life Time O_2/CO_2



(e) Particle Temperature O_2/N_2



(f) Particle Temperature O_2/CO_2

Figure 3 Compared particle ignition time, particle life time and particle temperature versus varied oxygen concentration under both N_2 and CO_2 background gas for coal DECS-11.

it is shown that the numerical results match the experimental data well.

Figures 3(a)-3(f) present the same compared information of coal DECS-11. The ignition delay time is spotted nicely according to Figures 3(a) and 3(b). Figures 3(c)-3(f) show that the numerical results of particle life time and particle temperature match the experimental data only with slight errors.

It is clear from the results shown in Figures 2 and 3, that there is a good agreement between the results of numerical simulations and experimental data. Hence, it can be concluded that the numerical model is valid.

Evolution of Chemical Species Concentration

Burning of a single particle in the experiments [1,2] resulted in very small amount of chemical species. Experimental measurement of these amounts is extremely hard. Yet, without knowing the evolution of chemical species concentration, our knowledge of combustion process will be incomplete. To address this, numerical simulations can be utilised to predict the details of the single coal combustion process.

The mass-averaged mole fraction of selected species volatile (hv_vol), H_2O, CO, and H_2 versus time after particle release of coal DECS-11 particle burning in 20% O_2 and 80% N_2, 100% O2, 40% O_2 and 60% CO_2 gas atmosphere are shown in Figure 4-6.

When the coal particles combust in O_2/N_2 gas atmospheres (Figure 4), the volatile appeared since the coal particle was injected into the reactor and the amount kept increasing till the peak. Further, the volatile reacted with oxygen to produce H_2O and CO_2. When all the volatile was consumed completely, the amount of H_2O became stable. The species CO, H_2 appeared when the coal particle was ignited. The amount of H_2 kept increasing during the coal combustion process and then became stable when the coal particle burned out. The amount of CO began decreasing when the rate of consuming CO was higher than producing CO, and finally all CO turned to CO_2. The changing trends of these species meet the combustion mechanism well.

When the coal particles burn in O_2/CO_2 gas atmospheres, based on the coal combustion mechanism described before, the volatile reacted with oxygen very early, and then the formation and consume of volatile competed. Hence there were two peaks of mole fraction of volatile (Figure 5). For other species, H_2O kept increasing until the volatile combust totally, and H2 appeared when the particle was ignited and reached maximum when the particle burn out, and CO produced during coal combustion reacted with oxygen and formed CO_2 at last.

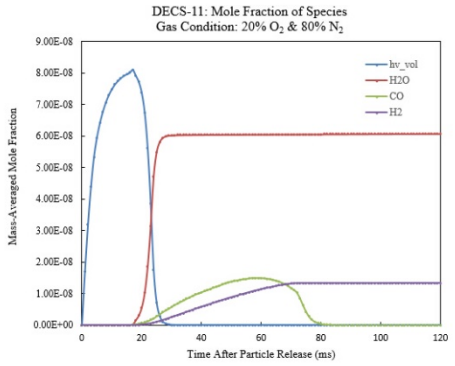


Figure 4 Mass-averaged mole fraction of selected species (hv_vol, H_2O, CO, H_2) versus time after particle release of coal DECS-11 particle burning in 20% O_2 and 80% N_2 gas atmosphere.

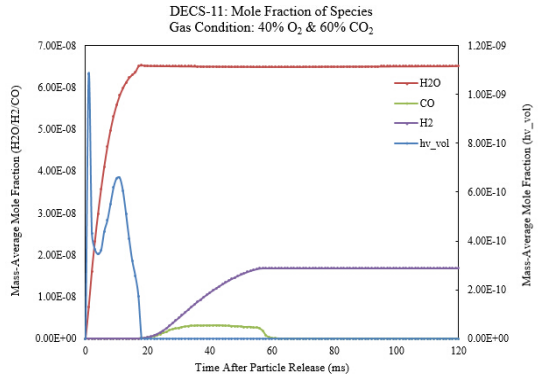


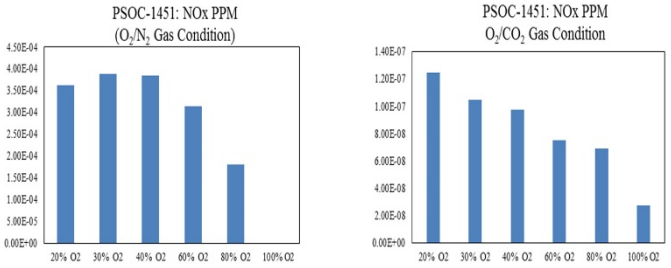
Figure 5 Mass-averaged mole fraction of selected species (hv_vol, H_2O, CO, H_2) versus time after particle release of coal DECS-11 particle burning in 40% O_2 and 60% CO_2 gas atmosphere.

Results of NO_x PPM

NOx concentration was not measured during experiments. Based on the valid numerical model, the predictions of NO emissions of both two kinds of coal in different oxygen mole fraction gas atmosphere were done by numerical simulations. Results are presented in Figure 6 and Figure 7. The two kinds of coal shared the same trends for all runs.

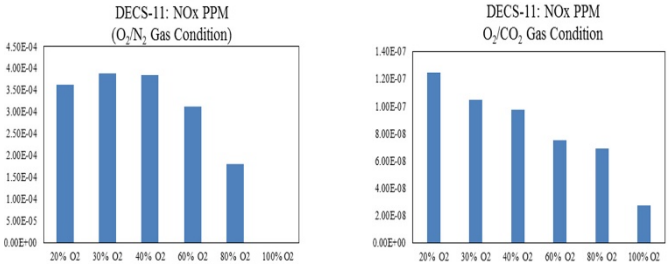
As only one single particle is burned in each case, the NO_x emissions produced by fuel-NO_x is much lower than thermal-NO_x. Therefore, the NO_x concentration is lower when coal particles burned under O_2/CO_2 gas conditions than O_2/N_2 gas conditions.

When the coal particles combust in O_2/N_2 gas conditions, the NO_x concentration increases when the mole fraction of oxygen increases from 20% to 30% and 40%. However, when the mole fraction of oxygen exceeds 50%, the NO_x concentration decreases when the mole fraction of oxygen increases. While the coal particles combust in O_2/CO_2 gas conditions, the NO_x concentration keeps decreasing when increasing the mole fraction of oxygen. NO_x emissions formed from fuel-NO_x are greatly influenced by fuel temperature and burnout time. Therefore when the particle life time decreases and particle temperature increases along with increscent oxygen concentration, the NOx concentration descends when combusting in O2/CO2 gas conditions.



(a) NO_x PPM O_2/N_2 (b) NO_x PPM O_2/CO_2

Figure 6 NO_x PPM for coal PSOC-1451 at T = 200 ms (Time After Particle Release)



(a) NO_x PPM O_2/N_2 (b) NO_x PPM O_2/CO_2

Figure 7 NO_x PPM for coal DECS-11 at T = 200 ms (Time After Particle Release)

CONCLUSIONS

Combustion of single coal particles (PSOC-1451 and DECS-11) was modelled numerically, existing experimental data were used to validate the simulation. The predicted results for the two kinds of coal featured a good agreement with the experimental data in terms of the particle ignition time, particle life time and particle temperature versus varied oxygen concentration under both N_2 and CO_2 background gas. Further, detailed changing trends of gas species were investigated in this study. Hence, the established model worked successfully and could be a useful predictive tool for coal combustion.

The NO emissions of both two kinds of coal in different oxygen mole fraction gas atmosphere were predicted. The two kinds of coal shared the same trends for all conducted simulations. The NO_x concentration was lower when coal particles burned under O_2/CO_2 gas conditions than O_2/N_2 gas conditions. When the coal particles combust in O_2/N_2 gas conditions, the NO_x concentration increased along with increscent oxygen concentration when the mole fraction of oxygen below 40%, and decreases when the mole fraction of oxygen exceeds 60%. On the other hand, the coal particles combusted in O_2/CO_2 gas conditions, the increase of the mole fraction of oxygen leaded to the decrease of NO_x concentration.

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REFERENCES

[1] Khatami R., Stivers C., Levendis L.A., Ignition characteristics of single coal particles from three different ranks in O2/N2 and O2/CO2 atmospheres, Combustion and Flame, vol 159, 2012, pp. 3554-3568.

[2] Maffei T., Khatami R., Pierucci S., Faravelli T., Ranzi E., Levendis L.A., Experimental and modelling study of single coal particle combustion in O2/N2 and Oxy-fuel (O2/CO2) atmospheres, Combustion and Flame, vol 160, 2013, pp. 2559-2572.

[3] Williams A, Backreedy R, Habib R, Jones JM, Pourkashanian M., Modelling coal combustion: the current position, Fuel, vol 81, 2002, pp. 605-618.

[4] Energy outlook 2012. International Energy Agency; 2012.

[5] Buhre B.J.P., Elliott L.K., Sheng C.D., Gupta R.P., Wall T.F., Oxy-fuel combustion technology for coal-fired power generation, Progress in Energy and Combustion Science, vol 31, 2005, pp. 283–307.

[6] Cao H.L., Sun S.Z., Liu Y.H., Wall T.F., Computational fluid dynamics modeling of NOx reduction mechanism in oxy-fuel combustion, Energy Fuels, vol 24, 2010, pp. 131-165.

[7] Kim C., Lior N., A numerical analysis of NOx formation and control in radiatively/conductively-stabilized pulverized coal combustors, Chemical Engineering Journal, vol 71, 1998, pp. 221-231.

[8] Hayhurst A.N., Vince I.M., Nitric oxide formation from N2 in flames: The importance of “prompt” NO, Progress in Energy and Combustion Science, vol 6, 1980, pp. 35-51.

[9] Benim AC, Epple B, Krohmer B. Modelling of pulverised coal combustion by a Eulerian-Eulerian two-phase flow formulation, Progress in Computational Fluid Dynamics, vol 6, 2005, pp. 345–61.

[10] Spliethoff H, Power generation from solid fuels, Heidelberg Dordrecht, London, New York: Springer; 2010.

[11] Rathnama R., Elliotta L., Walla T.F., Liua Y.K., Moghtaderib B., Differences in reactivity of pulverised coal in air (O2/N2) and oxy-fuel (O2/CO2) conditions, Fuel Processing Technology, vol 90, 2009, pp. 797-802.

[12] Scheffknecht G., Al-Makhadmeh L., Schnell U., Maier J, Oxy-fuel coal combustion—A review of the current state-of-the-art, International Journal of Greenhouse Gas Control, vol 5, 2011, pp. S16-S35.

[13] Brix J., Jensen P.A., Jensen A.D., Coal devolatilization and char conversion under suspension fired conditions in O2/N2 and O2/CO2 atmospheres, Fuel, vol 89, 2010, pp. 3373-3380.

[14] Borrego A.G., Alvarez D., Comparison of chars obtained under oxy-fuel and conventional pulverized coal combustion atmospheres, Energy Fuels, vol 21, 2007, pp. 3171-3179.

[15] Okazaki K., Ando T., NOx reduction mechanism in coal combustion with recycled CO2, Energy, vol 22, 1997, pp. 207-215.

[16] Hu Y.Q., Kobayashi N., Hasatani M., Effects of coal properties on recycled-NOx reduction in coal combustion with O2/recycled flue gas, Energy Conversion and Management, vol 44, 2003, pp. 2331-2340.

[17] Dhungel, B., Maier, J., Scheffknecht, G., Emission behavior during oxy-coal combustion, AIChE 2007 Annual meeting, Salt Lake City, UT, November 4, 2007.

[18] Mackrory, A. J., Lokare, S., Baxter, L. L., Tree, D. R., An investigation of nitrogen evolution in oxy-fuel combustion, 32rd International Technical Conference on Coal Utilization & Fuel Systems, Clearwater, FL, June 10-15, 2007.

[19] Kuffa M., Paul M.C., Janicka J., Combustion processes of biomass in a fluidized bed: A review and results of CFD modelling, In: Paul MC, editor. Soot: sources, formation and health effects, USA: Nova Science, 2012, pp. 243–80.

[20] Oevermann M., Gerber S., Behrendt F., Numerical simulation of wood gasification in a fluidized bed reactor using Euler–Euler modelling, Proceedings of the 4th European combustion meeting, 2009.

[21] Chui E.H., Douglas M.A., Tan Y., Modeling of oxy-fuel combustion for a western Canadian sub-bituminous coal, Fuel, vol 82, 2003, pp. 1201–1210.

[22] Wang L., Haworth D.C., Turns S.R., Modest M.F., Interactions among soot, thermal radiation, and NOx emissions in oxygen-enriched turbulent nonpremixed flames: a computational fluid dynamics modeling study, Combustion and Flame, vol 141, 2005, pp. 170–179.

[23] Smith T.F., Shen Z.F., Friedman J.N., Evaluation of coefficients for the weighted sum of gray gases model, Journal of Heat Transfer, vol 104, 1982, pp. 602–608.

[24] Fluent Inc., ‘‘Fluent 15.0 user’s guide’’; 2014.

[25] Chen C.X., Horio M., Kojima T., Numerical simulation of entrained flow coal gasifiers. Part I: modeling of coal gasification in an entrained flow gasifier, Chemical Engineering Science, vol 55, 2000, pp. 3861-3874.

[26] Mayers A.M., The rate of reduction of carbon dioxide by graphite, Journal of the American Chemical Society, vol 56, 1934, pp. 70–76.

[27] Howard J.B., Williams G.C., Fine D.H., Kinetics of carbon monoxide oxidation in postflame gases, Proceedings of 14th symposium (Interational) on combustion, vol 14, 1973, pp. 975–986.

[28] De Soete G. G., Overall reaction rates of NO and N_2 formation from fuel nitrogen, 15th Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, PA, vol 15, 1975, pp. 1093-1102.